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AFOSR-TR-83-0637 AFOSR-81-0091

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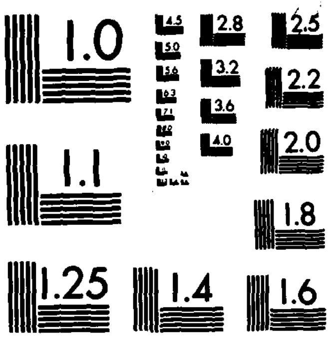

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REPORT DOCUMENTATION PAGE

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1. REPORT NUMBER AFOSR-TR- 83-0637	2. GOVT ACCESSION NO. AD-A131 661	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Strong Coupling Effects on Bound States in Plasmas		5. TYPE OF REPORT & PERIOD COVERED Progress Report (Interim) Feb. 1, 1982 thru Jan. 31, 1983
		6. PERFORMING ORG. REPORT NUMBER
AUTHOR(s) Gabor J. Kalman		8. CONTRACT OR GRANT NUMBER(s) AFOSR 81-0091
PERFORMING ORGANIZATION NAME AND ADDRESS Boston College Chestnut Hill, MA 02167		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2301/A8
11. CONTROLLING OFFICE NAME AND ADDRESS AFOSR/NP Bolling AFB, DC 20332		12. REPORT DATE March, 1983
		13. NUMBER OF PAGES 11
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

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18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Dense plasmas, strong coupling, bound states, ionization, Thomas-Fermi, dielectric function, phase-transition, critical curve.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Further progress in the areas of (1) kinetics and response of strongly coupled multi-component plasmas, (2) study of plasma phase transition and determination of the degree of ionization of a dense plasma, (3) generalization of the Thomas-Fermi-Debye-Huckel scheme for strongly coupled plasmas with atoms and ions, is reported: (1) A multi-species formalism has been worked out. 2 ~~(2)~~ Details of the phase transition and of the critical curve have been found. 3 ~~(3)~~ Relationship to other works has been studied.

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PROGRESS REPORT II

Grant AFOSR 81-0091

STRONG COUPLING EFFECTS ON BOUND STATES IN PLASMAS

March, 1983

I. RESEARCH WORK

Research in the report period continued along the lines indicated in Progress Report I, encompassing the following areas:

1. The analysis of the kinetics of strongly coupled two-component plasmas.
2. Study of the ionization equilibrium in a strongly coupled plasma medium.
3. Setting up a scheme appropriate for the study of the energy levels and of the ionization potential of atoms and ions in a strongly coupled plasma medium.

1. A convenient method to analyze the kinetics of strongly coupled plasmas is by way of partial response functions. This method was originally suggested by Singwi and Vashista[1] and then further analyzed and extended by Golden and Kalman[2]. However, attempts to use this approach for concrete calculations have been frustrated by the apparent complexity and unwieldiness of the formalism. We have recently succeeded to cast the formalism in a much simpler language by using matrix description in "species-space". By exploiting this new formalism we have already obtained some new and important results: (a) we have found that at least one of the ion-ion pair correlation functions in a multi-ion system exhibits an oscillatory behavior for arbitrary small coupling; (b) we have shown that if quantum and proximity corrections are taken into account in the interaction potential - which make the A-B interaction different from the A-A interaction (apart from scale), - the dielectric function exhibits a qualitatively new behavior; (c) by examining the structural features of the well-known Totsuji-Ichimaru approximation scheme for multi-species systems, we have discovered that it violates an important symmetry requirement and therefore its applicability to multi-species systems is doubtful.

These results have been incorporated in a paper addressing itself primarily to the basic formalism (publication (A)); further papers on the results listed above are in the process of preparation.

Another aspect of our research is based on an approximation scheme (the Golden-Kalman (GK) approach)[3] which combines the plasma kinetic equations with nonlinear fluctuation-dissipation relations. The physical transparency and mathematical tractability of the resulting chain of response function equations, which has already provided a very good qualitative description of one-component plasma collective modes in the strong coupling regime[3], leads us to believe that the GK procedure will be equally effective in the treatment of the corresponding multi-component plasma problem. Until recently, the needed fluctuation-dissipation relations have been lacking.

These relations have now been established by us for both binary ionic mixtures and fully ionized ion-electron plasmas. Our principal frequency domain result links a single three-point dynamical structure function to a combination of nonlinear partial response functions. This important advance in equilibrium statistical mechanics takes us one step closer to acquiring information about transport processes in the more realistic bound state plasmas, for it will now be possible to go ahead with the formulation of an approximation scheme leading to a dielectric response function description of collective modes in fully ionized multi-component plasmas. These results are given in publication (B).

Works listed under (C) and (D) deal with the problem of plasma oscillations in strongly coupled systems. Plasma oscillations are expected to reach a high level of excitation ($\sim\gamma$) for strong coupling. The ensuing dynamical perturbation on the bound states becomes substantial and the knowledge and understanding of the precise plasmon spectrum under these circumstances is essential.

(C) analyzes the relationship between perturbation theoretic and the non-perturbative GK approach. This latter method was applied some time ago[3] to the problem of plasmon dispersion and gave very good agreement with molecular dynamics computer simulations[4] as far as the plasmon dispersion was concerned, but the agreement with the width of the plasmon peak was rather poor. An improvement of our original approach described in (D) now has provided a remarkably good agreement in this connection as well, including the reproduction of the non-monotonic γ-dependence of the width. To the best of our knowledge this is the first successful theoretic description of this unexpected behavior.

2. The standard method for determining the degree of ionization in a plasma medium is through the use of the Saha-equation. However, the Saha-equation, based on a model of a gas composed of independent particles, becomes quite unreliable at high densities. The main effects ignored by the Saha equation treatment are (i) the proximity effect, and (ii) the depression of the ionization potential, which itself consists of the depression of the continuum and of the lifting of the bound states due to screening. We have developed and analyzed a model which shows the effect of the latter. The influence of the medium on the atom is described through the replacement of the intra-atomic potential by a screened Debye potential where the screening constant $\kappa = (4\pi e^2 n\beta)^{1/2}$ depends on the free electron density. Increasing values of κ cause the disappearance of high-lying bound states, leading to the elimination of the last bound state at $\kappa a \approx 1.1$ (a = Bohr-radius)[5]. Consequently, ionization becomes easier, and the calculated degree of ionization is substantially above the simple Saha result. Moreover, as more electrons

become free, the ionization potential is further depressed an an avalanche develops generating a sudden phase-transition-like transition from the weakly ionized to a highly ionized state. We have used the recent analytic approximation given by Green[6] to describe the bound states in a screened potential. The Saha equation was modified by using the Larkin correction[7] for the partition function. The resulting rather complex self-consistency condition for the degre of ionization was solved numerically. Detailed computer work has been performed recently with parameters pertaining to H-plasmas in a wide range of densities, up to the degeneracy limit. We have found the phase-diagram in the density-temperature plane, with a critical point in the vicinity of $T_c = 3$ eV, $n_c = 3 \times 10^{23}$ cm^{-3}. These results are described in publication (E). Further works on ions with higher Z values, and on the effect of the electron degeneracy are in progress.

3. There are a number of methods available for the study of the dynamics of an atom or ion immersed in an ionized medium[7]. The Thomas-Fermi (TF) method combines relative simplicity with excellent qualitative descriptive capability. While the TF scheme and its refinement have been employed to the problem on hand, the approaches used are appropriate for weakly coupled situations and not for the case of strong coupling. The scheme we have worked out is intended to include specific strong coupling effects and is summarized below.

- The system is considered to consist, for the purpose of the TF equation, of three species:

  (i) N_i classical nuclei of charge Z,

  (ii) $N_e = N_i X$ hot, classical, "free" electrons, and

  (iii) $N_b = N_i Y$ ($Y=Z-X$) degenerate bound electrons.

- The potential around a chosen nucleus is determined by the Poisson-equation with the g_{ei} and g_{ii} providing the density distribution of the surrounding particles.
- For the purpose of the calculation of the correlation functions the system consists of
  - (i) N_i ions of charge X and
  - (ii) N_e hot classical, "free" electrons, interacting through the effective potentials Φ_{ee},, Φ_{ii} and Φ_{ei}, such that $Z > Z_{eff} > X$.
- $Z_{eff,\ i}$ and $Z_{eff,\ e}$ are to be determined by the integrated charge densities of the bound electrons only.
- The correlation functions g_{ee} and g_{ei} are now to be determined by using one of the strongly coupled static plasma schemes-either the mean field theories, or HNC.
- Finally X is to be determined by calculating the free energy of the system and minimizing it with respect to X.

The salient feature of this scheme is that it applies the philosophy of the TF-DH (Debye-Huckel) method, but replaces the DH distribution with the correlation functions appropriate for strong coupling. In turn, the correlation functions depend on the effective potentials.

We have prepared a survey of the earlier TF and TF-DH works, starting with the early works of Feynman, Metropolis and Teller[8] and Latter[9] through the more recent works of Rozsnyai and Alder[10] and More and Skupsky[11], which we plan to make available as a Technical Report. The superiority of our scheme, as outlined, over the existing approaches is quite convincing.

There are a number of theoretical problems which have to be clarified before detailed numerical work can be performed:

(i) the proper definition of the chemical potential and chemical equilibrium for the two-electron mixture;

(ii) the behavior of the mean field theories for a multi-species system (see above);

(iii) the correct combination of the mean field theory approach with the TF scheme.

These questions are presently being investigated.

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II. FUTURE PLANS

We will continue to examine the three major problem areas listed above, with increased emphasis, however on topics (2) and (3), since the main objective of (1), namely the extension of the ocp formalism to the case of the multi-species systems has been accomplished. As to (2), we will include quantum (degeneracy) effects in the deformation of the phase diagram and will generalize for arbitrary Z values. Furthermore, we will attempt to analyze the depression of the continuum (as contrasted to the lifting of the bound states) - which is a rather difficult problem. As to (3), we hope to be able to clarify the pending theoretical problems and to start actual numerical calculations.

A further topic to be investigated is the effect of plasma oscillations on the bound states. We will analyze the level of oscillations from the available computer simulation data and will examine the possibility of the merging of the continuum with the high-lying bound states.

III. PUBLICATIONS AND PRESENTATIONS

(February 1, 1982 through January 31, 1983)

A. G. Kalman and K.I. Golden: Theory of Partial Response Function in Plasmas, to be submitted to Phys. Rev. A.

B. K.I. Golden and Lu De-xin: Dynamical Three-Point Correlations and Quadratic Response Functions in Binary Ionic Mixture Plasmas, J. Stat. Phys. 29, 281 (1982).

C. P. Carini, G. Kalman and K.I. Golden: Exact Dynamical Polarizability for One-Component Classical Plasmas, A26, 1686 (1982).

D. P. Carini and G. Kalman: Plasmon Damping and Dispersion for Strong Coupling, to be submitted to Phys. Lett.

E. G. Kalman, Ruo-Xian Ying and R. Hogaboom: Ionization Phase Transitions for Dense Plasmas, Abstract accepted for the 1983 Conference on Plasma Science, May 23-25, 1983 San Diego, CA.

F. G. Kalman: Nonlinear Response Functions and Collective Modes in a Strongly Coupled Plasma, Statistical Mechanics of Ionic Matter, Los Houches, France April 1982, unpublished.

G. G. Kalman: Dynamical Processes in Strongly Coupled Plasmas, invited paper, 2nd Int. Conf. on Non-Ideal Plasmas, Wustrow, DDR, October 1982, unpublished.

The works listed below were sponsored by an earlier AFOSR Grant; they appeared, however, during the present report period.

H. K.I. Golden and G. Kalman: Fluctuation-Dissipation Relations and the Velocity Average Approximation, Ann. Phys. (N.Y.), 143, 160 (1982).

I. K.I. Golden and G. Kalman: Moment Expansion of the Kinetic Equation and its Application to Strongly Coupled Plasmas, Phys. Rev. A26, 631 (1982).

Dr. G. Kalman was invited lecturer at the NATO Workshop on the Statistical Mechanics of Ionic Matter, Les Houches, April 1982; Dr. K. Golden (Consultant) was invtied lecturer at various institutions in the People's Republic of China, and at universities in Australia in the summer of 1982; Dr. G. Kalman was invited lecturer at the 2nd International Meeting on Non-Ideal Plasmas, Wustrow, DDR; Dr. G. Kalman is the convener of a session on strongly coupled plasmas on behalf of the Organizing Committee for the XVIth International Conference on Ionization Phenomena in Gases.